We are thankful to Prof. D. Sharma for providing experimental facilities and to Prof Suresh Chandra for helpful suggestions.

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Indian J. Phys. **47**, 380-382 (1973)

Pressure and ionic mass dependence of the superconducting transition temperature for simple metals : A pseudopotential calculation.

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(*Received* 26 *July* 1972, *revised* 29 *September* 1972)

Recently Gupta & Tripathi (1970, 1971a) have modified the Harrison's model pseudopotential and used it to study the various harmonic, thermal and superconducting properties of many simple metals. While investigating the superconducting transition temperature they found (Gupta & Tripathi 1971b) that b.c.c. lithium should be superconductor below 1.2°K approximately. There is no experimental evidence to support this result. Also lithium undergoes a change of phase at a higher temperature. In the present communication we have investigated, using the modified potential, the pressure dependence of the superconducting transition temperature (T_c) of three simple metals, Li, Al and Pb, and its ionic mass dependence for the last two metals. The results are found to be in fair agreement with the experiments and with the values calculated by other workers.

The form of the potential in the q space is .

$$W(q) = -\frac{1}{\Omega_0}\left[-\frac{4\pi Ze^2}{q^2} + \frac{\beta \exp(-q\gamma_c)}{(1+q^2\gamma_c^2)^2}\right] \quad \ldots (1)$$

where β and γ_c are two arbitrary parameters. The method of determination of these and their values for the metals under study are given in earlier papers by Gupta & Tripathi. (1970, 1971a, 1971b)

The expression for pressure dependence of T_c following McMillan (1968) can be written as :

$$\frac{d \ln T_c}{dP} = \frac{d \ln \Theta_D}{dP} - 1.04\left[\frac{0.62\mu^* - 1 - \mu^*}{\{\lambda - \mu^*(1+0.62\lambda)^2\}}\right]\frac{d\lambda}{dP} \quad \ldots (2)$$

where $\mu^* = \mu/\{1+\mu \ln (E_F/k\Theta_D)\}$

$$\mu = \frac{1}{\pi k_F}\int_0^{2k_F}\frac{dq}{q\epsilon(q)} \quad \text{and} \quad \ldots (3)$$

$$\lambda = \frac{m\Omega_0}{4\pi^2 k_F M k^2 \Theta_D^2}\int_0^{2k_F}\frac{q^3\omega^2(q)}{\epsilon^2(q)}\,dq.$$

For a detailed discussion of the expressions the reader is referred to Gupta & Tripathi (1971b) and McMillan (1968)

We have considered μ (the spherical average of the fully screened Coulomb interaction between electrons over the Fermi surface) to be independent of pressure as no information is available for the pressure dependence of Fermi energy, dielectric constant and other parameters on which it depends. Also for the pressure dependence of λ we take

$$\frac{d\lambda}{dP} = -2\lambda\frac{d \ln \Theta_D}{dP}. \quad (4)$$

The pressure dependence of other quantities in λ are neglected following McMillan (1968, Section V of the paper). He shows that I_{ν_L} which depends on the electron-ion potential is only weakly dependent on pressure. The error therefore, introduced in our calculations, by this approximation, are of minor importance in the final results. Also

$$\frac{d \ln \Theta_D}{dP} = \chi\frac{d \ln \Theta_D}{dV} = \chi\gamma \quad (5)$$

where χ and γ are compressibility and Grüneisen constant respectively.

Using eqns. (4) and (5) the eqn. (2) becomes

$$\frac{d \ln T_c}{dP} = \chi\gamma\left[1 + \frac{2.08\lambda(0.62\mu^* - 1 - \mu^*)}{\{\lambda - \mu^*(1+0.62\lambda)\}^2}\right] \quad (6)$$

The ionic mass dependence of T_c is considered through the dependence of Θ_D on M. The experimental evidence for this type of interaction was first provided by Maxwell (1950) and Reynolds *et al* (1950). Who measured T_c as a function of the mean mass of different isotopes for a few superconductors. If Coulomb pseudopotential μ^* is small then one has $T_c \propto M^{-\frac{1}{2}}$ (as $\Theta_D \propto M^{-\frac{1}{2}}$), but when μ^* is appreciable then in general $T_c \propto M^{-\alpha}$. The value of α is a measure of the Coulomb pseudopotential and can be written as .

$$= \frac{1}{2}\left[1 - \left[\frac{(1+0.62\lambda)\mu^{*2}(1+\lambda)(1.04)}{\{\lambda-\mu^*(1+0.62\lambda)\}^2}\right.\right. \tag{7}$$

Using expressions (6) and (7) the pressure dependence of T_c for Li, Al and Pb and the ionic mass dependence of T_c for Al and Pb have been calculated with the modified form of the potential (1). The results are presented in table 1. For

Table 1. The theoretical values and comparison with experiments

Metal	$d \ln T_c/dp \times 10^{-6}$			α		
	Present Authors	Experimental Reynolds *et al* (1950)	Coulthard (1970)	Present Authors	Experimental Reynold (1950)	Garland (1963, 1967)
Li	−108.2	—	—	—	—	—
Al	−29.75	−22	−(20±3)	0 368	—	0.37
Pb	−7 12	−5.3	−(1±4)	0 482	0 48	0 485

comparison, the theoretical results ($d \ln T_c/dP$) of Coulthard (1970) and of Garland (1963, 1967) are quoted along with the experimental ones of Smith & Chu (1967). Our value of $d \ln T_c/dp$ is in better agreement with the experiment than that obtained by Coulthard in the case of Pb but for Al we get only a qualitative agreement. For Li no comparison could be made. The computed value of α is also in good agreement with experiment for Pb and with that calculated by Garland. For Al no experimental value is available but our value is in good agreement with that of Garland. It seems that for the pressure dependence of T_c to be a very informative parameter, more theoretical and experimental works are necessary on the pressure dependence of normal state properties so that the approximations made in the theory can also be accounted for.

One of the authors (GB) is grateful to the CSIR (India) for financial assistance.

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